

The BCS theory of superconductivity revisited: quasiparticle imbalance in equilibrium and multiple solutions of the energy gap equation

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We examine the equilibrium solutions of the BCS theory of superconductivity in the low temperature limit, allowing the attraction band to be asymmetric with respect to the chemical potential of the system μ_R . If we denote by μ the middle of the attraction band, we observe that the superconducting phase is formed only if $|\mu_R - \mu| < 2\Delta_0$, where Δ_0 is the energy gap at zero temperature in the standard BCS theory. If $|\mu_R - \mu| < 2\Delta_0$, the system of equations which give the energy gap has two solutions for each value of $\mu_R - \mu$: one with $\Delta(T=0) = \Delta_0$ and another one, with $\Delta(T=0) < \Delta_0$ ($\Delta(T=0)$ is the energy gap at 0 K). If $0 < |\mu_R - \mu| < 2\Delta_0$, a quasiparticle imbalance appears in equilibrium. In the “standard BCS limit,” which is $\mu_R \rightarrow \mu$, beside the standard solution $\Delta(T=0) = \Delta_0$, we find another one, with $\Delta(T=0) = \Delta_0/3$ and nonzero quasiparticle population. The formalism takes into account in a consistent way the variation of the total number of particles with the population of the quasiparticle states.

INTRODUCTION

In Ref. [1], the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity [2, 3] has been revisited under the assumption that the attraction band is asymmetric with respect to the chemical potential of the system. This asymmetry changes dramatically the phenomenology of the superconducting phase: a quasiparticle imbalance appears in equilibrium, the energy gap and the critical temperature change, there are several solutions for the gap equation, and, most significantly, the normal metal-superconductor phase transition becomes of the first order. If the attraction band—i.e. the single-particle energy interval in which the pairing interaction is manifested—is denoted by $I_V \equiv [\mu - \hbar\omega_c, \mu + \hbar\omega_c]$ and the chemical potential is denoted by μ_R , then the standard BCS phenomenology is recovered only if $\mu = \mu_R$. If $\mu \neq \mu_R$, the energy gap and the populations of the quasiparticle energy levels are calculated by solving a system of integral equations. As we shall see further, this system may have several solutions at fixed temperature and chemical potential.

Quasiparticle imbalance in the context of the BCS theory have been reported before for non-equilibrium superconductors (see for example Refs. [4–8]). Such non-equilibrium situations can be described also by our approach, but here we focus only on equilibrium superconductivity.

Equilibrium quasiparticle imbalance [9–11] appears also in the model of hole superconductivity [12, 13], but the concept and the predictions of this model are, in many respects, very different from the BCS theory. We do not make here comparisons between different models.

The effect of pressure on the superconducting properties have been studied for example in Ref. [14], where a bell-shaped dependence of the critical temperature on the pressure applied to the sample was observed. If the

relative position of the chemical potential with respect to the middle of the attraction band can be monotonically changed by the applied pressure, then a similar dependence of the critical temperature would appear in our model also [1].

The paper is organized as follows. In the next section we present the basic equations, from Ref. [1]. In the third section we present the low temperature limit of these equations and their solutions. In the forth section we present the conclusions.

THE SELF-CONSISTENT SET OF EQUATIONS

For simplicity, we work in the quasicontinuous limit and we denote by $\epsilon^{(0)}$ the energy of the free electrons. If the attraction band (or the conduction band, if this is included into the attraction band) $I_V \equiv [\mu - \hbar\omega_c, \mu + \hbar\omega_c]$ is centered at μ , then we denote the chemical potential of the system by μ_R and we introduce the usual notation $\xi \equiv \epsilon^{(0)} - \mu$ (see Ref. [1] for details). If the density of states (DOS) is $\sigma(\epsilon^{(0)}) \equiv \sigma(\xi + \mu)$, then the energy gap Δ satisfies the equation

$$\frac{2}{V} = \int_{-\hbar\omega_c}^{\hbar\omega_c} \frac{1 - n_{\xi 0} - n_{\xi 1}}{\epsilon(\xi)} \sigma(\xi + \mu) d\xi, \quad (1a)$$

where V is the pairing interaction, $\epsilon \equiv \epsilon(\xi) = \sqrt{\xi^2 + \Delta^2}$ are the BCS quasiparticle energies and $n_{\xi i}$ are the populations of the quasiparticle states ($i = 0, 1$), given by the equation [1]

$$n_{\xi i} = \frac{1}{e^{\beta[\epsilon(\xi) - (\mu_R - \mu)(\xi - F)/\epsilon(\xi)]} + 1}, \quad (1b)$$

with the parameter

$$F \equiv \frac{\int_{-\hbar\omega_c}^{\hbar\omega_c} (1 - n_{\xi 0} - n_{\xi 1}) \frac{\xi}{\epsilon^3(\xi)} d\xi}{\int_{-\hbar\omega_c}^{\hbar\omega_c} \frac{(1 - n_{\xi 0} - n_{\xi 1}) d\xi}{\epsilon^3(\xi)}}, \quad (1c)$$

$\beta \equiv 1/(k_B T)$, and T is the temperature of the superconductor. The system (1) should be solved self-consistently, to determine the energy gap and the populations [1]. Introducing the dimensionless variables $x_F \equiv \beta F$, $x \equiv \beta \epsilon$, $y \equiv \beta \Delta$, and $y_R \equiv \beta(\mu_R - \mu)$, and assuming a constant density of states $\sigma(\xi + \mu) \equiv \sigma_0$, Eqs. (1) become

$$x_F = \frac{\int_y^{\beta \hbar \omega_c} \frac{(n_x - n_{-x}) dx}{x^2}}{\int_y^{\beta \hbar \omega_c} \frac{(1 - n_x - n_{-x}) dx}{x^2 \sqrt{x^2 - y^2}}}, \quad (2a)$$

$$n_x = \frac{1}{e^{x - y_R (\sqrt{x^2 - y^2} - x_F)/x} + 1}, \quad (2b)$$

$$n_{-x} = \frac{1}{e^{x - y_R (-\sqrt{x^2 - y^2} - x_F)/x} + 1}, \quad (2c)$$

$$\frac{1}{\sigma_0 V} = \int_y^{\beta \hbar \omega_c} \frac{1 - n_x - n_{-x}}{\sqrt{x^2 - y^2}} dx, \quad (2d)$$

where we wrote explicitly the populations for the positive and negative branches, namely $\xi = \sqrt{\epsilon^2 - \Delta^2}$ in Eq. (2b) and $\xi = -\sqrt{\epsilon^2 - \Delta^2}$ in Eq. (2c). Equations (2) are symmetric under the exchange $y_R \rightarrow -y_R$, $x_F \rightarrow -x_F$, and $\xi \rightarrow -\xi$. The total number of particles is [1]

$$N = N_\mu + 2\sigma_0 \int_{-\hbar \omega_c}^{\hbar \omega_c} \frac{\xi n_\xi}{\sqrt{\xi^2 + \Delta^2}} d\xi, \quad (3)$$

where N_μ (a constant) represents the number of single-particle states up to level μ , in the noninteracting system.

In Eqs. (2) we have a couple of parameters that we can set: $\mu_R - \mu$ and T or, equivalently, y_R and T . Once this set of parameters is chosen, the system has to be solved self-consistently. In some cases, it admits several solutions. To determine the number of solutions and their values, we start by analyzing the system in the low temperature limit and constant DOS.

LOW TEMPERATURE LIMIT AND CONSTANT DOS

We start from the system of Eqs. (2) and we discuss only the case $y_R > 0$. The solutions for $y_R < 0$ can be obtained from the solutions with $y_R > 0$, by the replacement $x_F \rightarrow -x_F$ and exchanging n_ξ with $n_{-\xi}$. We analyze the argument of the exponential function in the denominator of n_x and n_{-x} of Eqs. (2). If we write $n_x \equiv \{\exp[\beta m_x] + 1\}^{-1}$ and $n_{-x} \equiv \{\exp[\beta m_{-x}] + 1\}^{-1}$, then

$$m_x \equiv \frac{\Delta}{r} (r^2 - a\sqrt{r^2 - 1} + ab), \quad (4a)$$

$$m_{-x} \equiv \frac{\Delta}{r} (r^2 + a\sqrt{r^2 - 1} + ab), \quad (4b)$$

where $r = \epsilon/\Delta = x/y \geq 1$, $a = (\mu_R - \mu)/\Delta = y_R/y$, and $b = F/\Delta = x_F/y$. When $m_x > 0$, then

$\lim_{T \rightarrow 0} \beta m_x = \infty$ and $\lim_{T \rightarrow 0} n_x = 0$, whereas if $m_x < 0$, then $\lim_{T \rightarrow 0} \beta m_x = -\infty$ and $\lim_{T \rightarrow 0} n_x = 1$. Similarly, in the limit $T \rightarrow 0$, if $m_{-x} > 0$, then $n_{-x} = 0$ and if $m_{-x} < 0$, then $n_{-x} = 1$.

Let us now find the values of r for which $m_x < 0$ or $m_{-x} < 0$. In Eqs. (4) we denote $t \equiv \sqrt{r^2 - 1} \geq 0$ and we rewrite them as

$$m_x \equiv \frac{\Delta}{t^2 + 1} (t^2 - at + ab + 1), \quad (5a)$$

$$m_{-x} \equiv \frac{\Delta}{t^2 + 1} (t^2 + at + ab + 1), \quad (5b)$$

We can now see that m_x and m_{-x} may take negative values only if the discriminant of Eqs. (5), $D \equiv a^2 - 4ab - 4$, is positive. Then, the solutions for Eq. (5a) are

$$t_1 = \frac{a - \sqrt{a^2 - 4ab - 4}}{2} \text{ and } t_2 = \frac{a + \sqrt{a^2 - 4ab - 4}}{2} \quad (6)$$

whereas the solutions for Eq. (5b) are $t'_1 = -t_2$ and $t'_2 = -t_1$. Obviously, $t_2 > 0$ and $t'_1 < 0$. If we denote by $I_r \equiv (r_1, r_2)$, the interval on which $m_x(r) < 0$ (4a), then

$$r_2 \equiv \sqrt{t_2^2 + 1} = \sqrt{\frac{a}{2} (a - 2b + \sqrt{a^2 - 4ab - 4})} \geq 1. \quad (7a)$$

Since $t_1 \leq 0$ if and only if $ab \leq -1$, then

$$r_1 = \begin{cases} \sqrt{\frac{a}{2} (a - 2b - \sqrt{a^2 - 4ab - 4})}, & \text{if } ab > -1, \\ 1, & \text{if } ab \leq -1. \end{cases} \quad (7b)$$

Similarly, $I'_r \equiv (r'_1, r'_2)$ is the interval on which $m_{-x}(r) < 0$ (4b). Then $r'_1 = 1$ (since $t'_1 = -t_2 < 0$) and

$$r'_2 = \begin{cases} \sqrt{\frac{a}{2} (a - 2b - \sqrt{a^2 - 4ab - 4})}, & \text{if } ab < -1, \\ 1, & \text{if } ab \geq -1. \end{cases} \quad (7c)$$

For $r \in I_r$, $\lim_{T \rightarrow 0} n_x(T) = 1$, whereas for $r \in [1, \infty) \setminus [r_1, r_2]$, $\lim_{T \rightarrow 0} n_x(T) = 0$. Similarly, for $r \in I'_r$, $\lim_{T \rightarrow 0} n_{-x}(T) = 1$, whereas for $r \in [1, \infty) \setminus [r'_1, r'_2]$, $\lim_{T \rightarrow 0} n_{-x}(T) = 0$. We also observe that $I'_r \subset I_r$, because, if $t_1 \geq 0$, then $r_1 \geq 1$ and $I'_r = \emptyset \subset I_r$, whereas if $t_1 \leq 0$, then $r_1 = r'_1 = 1$ and $r_2 > r'_2$ (Eqs. 7a and 7c), which implies again $I'_r \subset I_r$. Using this observation we see that $f_n(x) \equiv n_{-x} - n_x$, which appears in the integrand in the numerator of Eq. (2a), is different from zero only if $x/y = r \in \text{Int}(I_r \setminus I'_r)$ (where $\text{Int}(\cdot)$ denotes the interior of an interval), whereas $f_d(x) \equiv 1 - n_{-x} - n_x$, which appears in the integrand in the denominator, is zero in the same interval. Furthermore, $f_d(x) = -1$, if $x/y = r \in I'_r$, and $f_d(x) = 1$, if $x/y = r \in (r_2, \infty)$.

Let us now calculate Δ and x_F . We introduce the notation $r_0 \equiv \sqrt{(a/2) (a - 2b - \sqrt{a^2 - 4ab - 4})} \geq 1$. If $ab \geq -1$, then, from Eqs. (2), we obtain

$$\frac{1}{\sigma_0 V} = \log \left(\frac{2\hbar \omega_c}{\Delta} \right) - \log \left(\frac{r_2 + \sqrt{r_2^2 - 1}}{r_0 + \sqrt{r_0^2 - 1}} \right), \quad (8a)$$

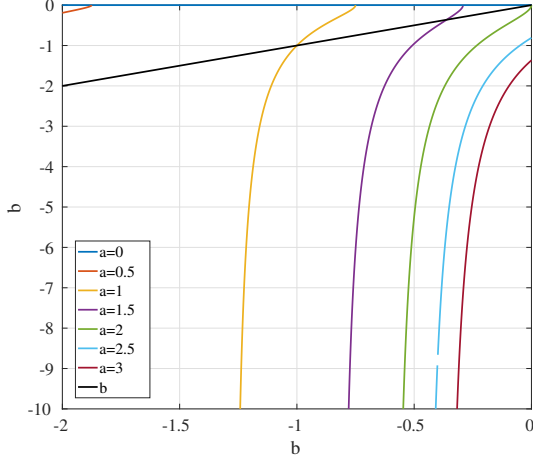


FIG. 1. (Color online) The r.h.s. of Eq. (8b), for $-1 \leq ab \leq 0$, continued by (9b), for $ab \leq -1$, plotted vs. b , for different values of a . The straight black line is b vs b .

$$b = \frac{\frac{1}{r_2} - \frac{1}{r_0}}{1 - \frac{\sqrt{r_2^2 - 1}}{r_2} + \frac{\sqrt{r_0^2 - 1}}{r_0}}, \quad (8b)$$

and we already observe that $b < 0$. From Eq. (8a) we can eliminate $1/(\sigma_0 V)$ and write

$$\frac{\Delta}{\Delta_0} = \frac{r_0 + \sqrt{r_0^2 - 1}}{r_2 + \sqrt{r_2^2 - 1}}, \quad (8c)$$

If $ab < -1$, then,

$$\frac{1}{\sigma_0 V} = \log\left(\frac{2\hbar\omega_c}{\Delta}\right) - \log\left(r_2 + \sqrt{r_2^2 - 1}\right) - \log\left(r_0 + \sqrt{r_0^2 - 1}\right), \quad (9a)$$

$$b = \frac{\frac{1}{r_2} - \frac{1}{r_0}}{1 - \frac{\sqrt{r_2^2 - 1}}{r_2} - \frac{\sqrt{r_0^2 - 1}}{r_0}}, \quad (9b)$$

Eliminating $1/(\sigma_0 V)$ from Eq. (9a) we write

$$\frac{\Delta}{\Delta_0} = \frac{1}{\left(r_0 + \sqrt{r_0^2 - 1}\right)\left(r_2 + \sqrt{r_2^2 - 1}\right)}. \quad (9c)$$

If $ab = -1$, then $r_0 = 1$ and Eqs. (8) and (9) give the same results, implying that the functions $b(a)$ and $\Delta(a)$ are continuous.

Numerical and analytical analysis of Eqs. (8) and (9) show that for $0 < a < 2$ there are two solutions (see Fig. 1): one with $b = 0$, $n_x(T = 0) = n_{-x}(T = 0) = 0$, and $\Delta(T = 0) = \Delta_0$, and another one, with $b < 0$ and $\Delta(T = 0) < \Delta_0$, whereas $n_x(T = 0)$ and $n_{-x}(T = 0)$ may take nonzero values for some values of x . For $a = 2$ (green curve in Fig. 1), only the solution with $b = 0$ remains, whereas for $a > 2$, Eqs. (8) and (9) have no solutions and the superconducting phase cannot be formed at $T = 0$.

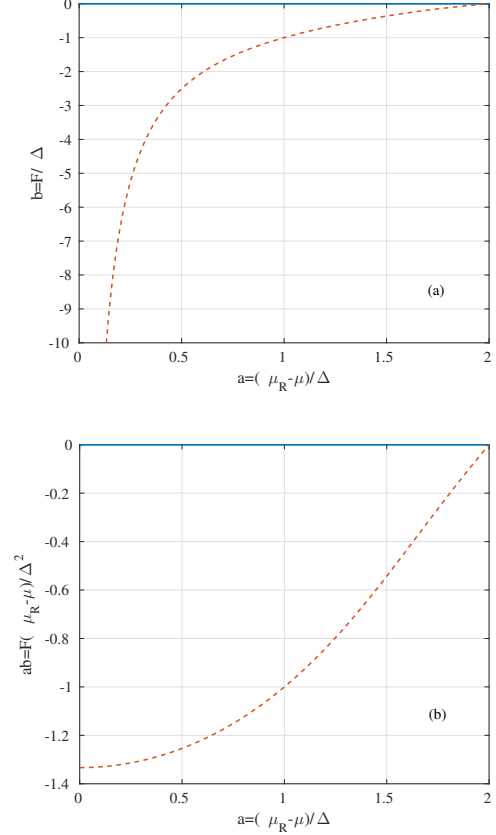


FIG. 2. In (a) are the solutions b vs a , obtained from Eqs. (8) and (9). There are two solutions, $b \equiv 0$ (solid blue line) and $b < 0$ (dashed red line). In (b) we plot the product ab vs a . For the negative function (dashed red line), $\lim_{a \searrow 0} ab = 4/3$.

The solutions $b(a)$, from Eqs. (8) and (9), are plotted in Fig. 2. We see that if $a < 1$, then $ab < -1$ (see Fig. 2 b). In this case, $n_x(T = 0) = 1$, for $r = x/y \in [1, r_2]$, and $n_{-x}(T = 0) = 1$, for $r = x/y \in [1, r_0]$. In the limit $a \searrow 0$, the product ab converges to a constant, which can be readily calculated from Eq. (9b), namely

$$\lim_{a \rightarrow 0} ab = -4/3. \quad (10)$$

For $a \in (1, 2)$, we have $ab \in (-1, 0)$ and $n_x(T = 0) = 1$, if $r = x/y \in (r_0, r_2)$, whereas $n_{-x}(T = 0) = 0$ for any r .

In Fig. 3 we plot $\Delta(T = 0)/\Delta_0$ for the two solutions of b plotted in Fig. 2 (a). For the solution $b \equiv 0$, $\Delta(T = 0) = \Delta_0$ for any x , whereas for the solution $b < 0$, $\Delta(T = 0) \leq \Delta_0$. Using Eqs. (9c) and (10) we obtain

$$\lim_{a \rightarrow 0} \Delta^{(b < 0)}(T = 0) = \Delta_0/3, \quad (11)$$

for the solution with $b < 0$.

Having the solutions for b and Δ , we can calculate the quasiparticle populations and the quasiparticle imbalance. For the solutions with $b = 0$, the situation is trivial: $n_x = n_{-x} = 0$ for any r . For $b < 0$, if

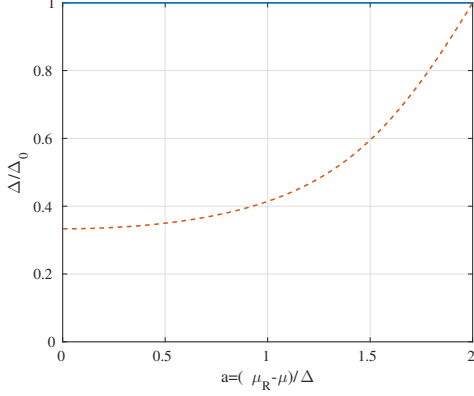


FIG. 3. The ratio $\Delta(T=0)/\Delta_0$ vs a , for the solutions of b plotted in Fig. 2.

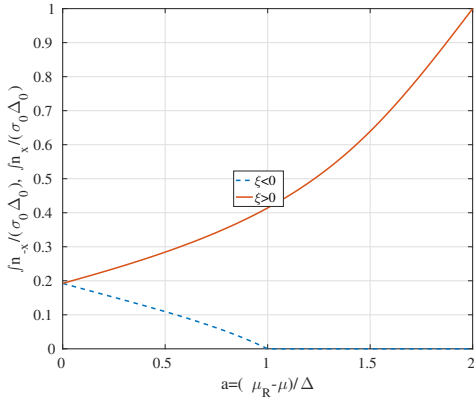


FIG. 4. (Color online) The total populations (integral over the ξ or ϵ , symbolically represented as a primitive) of the branches with $\xi < 0$ (blue dashed line) and $\xi > 0$ (red solid line), for the solutions with $b < 0$.

$1 < a < 2$, then $-1 < ab < 0$ and only the branch with $\xi > 0$ is populated for $\xi \in [\Delta\sqrt{r_0^2-1}, \Delta\sqrt{r_2^2-1}]$. If $0 < a < 1$, then $-4/3 < ab < -1$ and both branches are populated: the branch $\xi < 0$ is populated in the interval $\xi \in [-\Delta\sqrt{r_0^2-1}, 0]$, whereas the branch $\xi > 0$ is populated in the interval $\xi \in [0, \Delta\sqrt{r_2^2-1}]$. We plot these populations in Fig. 4 and we observe that the branch imbalance is non-zero for any $a > 0$, whereas $\lim_{a \nearrow 2} n_x/(\sigma_0\Delta_0) = 1$. When $a \searrow 0$, the population imbalance disappears, although $b \rightarrow -\infty$ and $\Delta \searrow \Delta_0/3$. This situation corresponds to $\mu_R = \mu$, $\Delta = \Delta_0/3$, and the population for each branch equal to $\sigma_0\Delta_0/(3\sqrt{3})$.

The total number of particles is given by Eq. (3). For the situation when $b \equiv 0$ and $\Delta = \Delta_0$, $n_x = n_{-x} = 0$ and $N = N_\mu$ for any a . In the case of solutions with $b < 0$,

from Eq. (3) we obtain

$$\frac{N - N_\mu}{2\sigma_0} = \int_{\Delta\sqrt{r_0^2-1}}^{\Delta\sqrt{r_2^2-1}} \frac{\xi d\xi}{\sqrt{\xi^2 + \Delta^2}} = \Delta(r_2 - r_0). \quad (12a)$$

If we define by N_{μ_R} the number of free-particle states up to μ_R , then

$$\frac{N - N_{\mu_R}}{2\sigma_0} = \frac{N - N_\mu}{2\sigma_0} - (\mu_R - \mu) = \Delta(r_2 - r_0 - a). \quad (12b)$$

For $a \in (0, 2)$, $N - N_\mu > 0$, whereas $N - N_{\mu_R} < 0$. For $a = 0$, $N - N_\mu = N - N_{\mu_R} = 0$, whereas for $a = 2$, $N - N_\mu = 0$ and $N - N_{\mu_R} = -4\sigma_0\Delta_0$.

Variation of particle number upon condensation may lead to charging effects, which will be discussed elsewhere. Nevertheless, we observe that if $a = 0$ (i.e. $\mu_R = \mu$), which corresponds to the standard BCS theory, the system of equations (2) have two solutions—not one—and in both, the charge neutrality is preserved. The first solution is the standard BCS result, with $\Delta(T=0) = \Delta_0$, whereas the other one corresponds to $\Delta(T=0) = \Delta_0/3$. In both solutions the branch balance is also preserved, although in the first case the populations of the quasiparticle states is zero, whereas in the other case the populations of both branches are equal to $\sigma_0\Delta_0/(3\sqrt{3})$ (see Fig. 4).

CONCLUSIONS

We analyzed the BCS formalism in the low temperature limit, under the assumption that the attraction band is asymmetric with respect to the chemical potential of the system μ_R . We denoted by μ the center of the attraction band and by Δ_0 the energy gap in the standard BCS theory. We observed that if $|\mu_R - \mu| > 2\Delta_0$, the system of equations (2), which gives the energy gap, has no solutions, so, in this case, the superconducting state cannot exist even at zero temperature. If $|\mu_R - \mu|/\Delta_0 \in (0, 2)$, the system (2) has two solutions: one with $\Delta(T=0) = \Delta_0$ and another one, with $\Delta(T=0) < \Delta_0$ (see Fig. 3) and a quasiparticle imbalance appears in equilibrium (see Fig. 4). It is interesting to note that in the limit $\mu_R \rightarrow \mu$, when the standard BCS theory should be obtained, the system (2) still has two solutions, one with $\Delta(T=0) = \Delta_0$ (as expected) and another one, with $\Delta(T=0) = \Delta_0/3$. In this case, for both solutions the quasiparticle imbalance disappears. Considering that electrons with momenta oriented along different directions do not interact with each-other, these solutions may even exist simultaneously in the same superconductor [15–18].

The change of the number of particles, when going from the normal metal state to the superconducting state

(Eqs. 12) would lead to charging effects if the Coulomb interaction is taken into account. Nevertheless, these effects do not influence the solutions for $\mu_R \rightarrow \mu$, since in this case the number of particles is conserved and $N_\mu = N_{\mu_R} = N$.

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